# Triply differential cross section and polarization correlations in electron bremsstrahlung emission

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We report results from a reformulation of the relativistic bremsstrahlung code of Tseng and Pratt. This permits calculation of the triply differential cross section $d^3\sigma$ of bremsstrahlung (electron-photon coincidence measurements) in electron scattering on neutral atoms and ions. The cross section $d^3\sigma$ is viewed as a more sensitive test of the theory, and predictions are needed for comparison with the more systematic and accurate experiments which are now being undertaken. The reformulation represents an extension of the previous code (which only calculated the doubly differential cross section), again utilizing partial-wave and multipole expansions in a screened potential within the independent particle approximation, but differently organizing their summation. The best previous predictions for the triply differential cross sections are due to Elwert and Haug, under assumptions less restrictive than Born approximation yet valid for high-$Z$ elements only at very high incident electron energy. While we confirm differences from the Elwert-Haug results, we do not see a systematic improvement in the agreement with the limited previous experimental data, and further experiments are awaited with interest. [S1050-2947(96)01606-X]

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## I. INTRODUCTION

The radiation of a photon as an electron scatters from an atom represents a fundamental process in which to study the electron-photon interaction in the field of the atom. While there are many experiments involving observation of the radiated photon or the outgoing electron, few exist in which both the electron and photon are observed. It is often argued that such a more complete measurement of a process offers a more stringent test of the description of the interaction [1]. Here we present some results for calculation of the triply differential cross section and polarization correlations for electron-atom bremsstrahlung. These calculations were performed using a relativistic partial-wave and multipole expansion of the relevant matrix elements, including all orders in the interaction of the electron with the potential of the atom (within the independent-particle approximation) and a first order interaction of the scattering electron with the emitted photon.

In a recent article [1] Nakel has given a comprehensive review of bremsstrahlung experiments thus far performed which involve coincident detection of both electron and photon. These experiments cover, sparsely, a broad range of atomic numbers at three incident electron energies (140 keV, 180 keV, and 300 keV). All the existing experiments use a coplanar geometry, with the photon emitted in the plane of electron scattering. There are no data for scattering from ions, and very few data from experiments involving polarized beams or observation of electron or photon polarization (''polarization'' experiments). In most cases the experimental error in cross sections is estimated to be greater than 10%.

Prior to the present work two relevant theoretical formulations were available: first Born approximation, due to Bethe and Heitler [2], and results of Elwert and Haug [3] using Sommerfeld-Maue wave functions [4]. The first Born approximation result (which includes a form factor for screened potentials), is expected to be valid when $\alpha Z/\beta \ll 1$ ($\alpha$ is the fine structure constant, $Z$ the atomic number, and $\beta$ the electron velocity in units of the velocity of light in vacuum) for both the incident and outgoing electron. Thus the region of validity of this approximation is limited to low-$Z$ elements with high incident and outgoing electron energies. The agreement of Born approximation with existing experiments is limited, even in such situations. (This possibly offers some assessment of the accuracy of the older experimental data.) As expected, substantial deviations of Born approximation from experiment have been seen for $Z>29$ at most electron energies. In an improved calculation Elwert and Haug utilized approximate Coulomb (Sommerfeld-Maue) wave functions to obtain formulas expected to be valid in the point Coulomb potential for $\alpha Z \ll 1$ at all energies, or for all $\alpha Z$ at sufficiently high incident and outgoing electron energy, and in suitable intermediate situations. Form factors are often included in these predictions to correct for screening effects. While showing some improvement over the Born approximation results for intermediate and high $Z$, significant differences are still seen between Elwert-Haug results and experiment, particularly for $Z=79$, which is outside the expected range of validity of the approximation for energies typical in the current experiments.

In this paper we report studies of the triply differential

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cross section based on a relativistic multipole and partial-wave expansion in a screened central potential. For the neutral atom potential we use the self-consistent field program described by Liberman *et al.* [5], but without a Latter tail. Our studies utilize an extension and reformulation of the previous multipole and partial-wave expansion method of Tseng and Pratt [6], which was successful for calculation of the doubly differential cross section, but which used techniques not easily applicable to the numerical problems of the triply differential cross section. The method [6] has thus far provided the best available calculations of the doubly differential cross section and associated polarization parameters [7].

In Tseng and Pratt's approach [6,8] the doubly differential cross section was calculated by writing the full triply differential cross section as a double sum over products of matrix elements, $\Sigma_{\mathscr{K},\mathscr{L}}\mathscr{M}^*_{\mathscr{K}}\mathscr{M}_{\mathscr{L}}$, where $\mathscr{K}(L,\kappa_i,\kappa_f)$ and $\mathscr{L}$ each represent values related to the angular momentum $(L)$ associated with the photon and the total angular momentum of the initial $(\kappa_i)$ and final $(\kappa_f)$ continuum states of the electron, i.e., a sixfold summation. Integration over outgoing electron angles to obtain the doubly differential cross section may be done analytically and collapses the double summation over the corresponding outgoing electron angular momentum, leaving no interference terms. Since there is no corresponding collapse when calculating the triply differential cross section (and related observables) all sums must be performed numerically. Such a computation would be difficult due to the large number of multipole and partial-wave terms required to obtain convergence. In this work we have instead summed the matrix elements numerically and then squared the sum, $|\Sigma_{\mathscr{L}}\mathscr{M}_{\mathscr{L}}|^2$, thereby reducing the number of summations to three. While this expression is mathematically identical to the triply differential form $\Sigma_{\mathscr{K},\mathscr{L}}\mathscr{M}^*_{\mathscr{K}}\mathscr{M}_{\mathscr{L}}$, it is much more convenient from a computational viewpoint.

In the following section we give a more detailed description of the theoretical method used in our computation and discuss tests of its accuracy. We discuss the respective merits of this formulation versus that of Tseng and Pratt in the calculation of various physical observables. In Sec. III we report some results from our calculations, including comparisons with simpler theories which confirm that in some circumstances there are large differences from the theory of Elwert and Haug, particularly for high-$Z$ elements. In preparation for comparisons with experiments now being undertaken [9], we have obtained some data corresponding to the existing experiments. In some cases, but not systematically, some improvement in the agreement of theory with these experiments is seen. More importantly, we hope that the availability of these more accurate predictions will encourage further precision experiments.

## II. THEORY

We follow the partial-wave and multipole expansion methods used by Pratt and Feng [7]. We first calculate the Dirac-Slater potential, then the partial waves of the initial and final electron states (of energy $E_1$ and $E_2$, respectively) in the potential, and with them the radial multipole matrix elements. However, we do not directly calculate the triply differential cross section and the 32 polarization coefficients in the manner discussed by Tseng [8], but rather we first calculate the full matrix element. Instead of utilizing the fact that the cross section is linear in initial and final electron spin and photon Stokes parameters, we utilize the fact that the matrix element is linear in the complex coefficients $(a^{\uparrow},a^{\downarrow})$ characterizing initial and final asymptotic electron spin states (defined in the rest frame of each electron) and the complex photon polarization coefficients $(\epsilon_+,\epsilon_-)$. In general we can expect this method to be preferable to the method developed by Tseng [8] when obtaining a totally differential observable. To calculate the triply differential cross section Tseng's method, since it does not utilize the information that the cross section can be written as a perfect square, would require double summations over both incident and outgoing electron partial waves and a double sum over allowed photon angular momenta: $(\Sigma_{\mathscr{K}\mathscr{L}}\mathscr{M}^*_{\mathscr{K}}\mathscr{M}_{\mathscr{L}})$. The method described here requires only a single summation over incident and outgoing electron partial waves and a single summation over photon angular momenta: $(|\Sigma_{\mathscr{L}}\mathscr{M}_{\mathscr{L}}|^2)$. However, the approach has the disadvantage that sums (or integrations) over quantities not observed will be performed numerically rather than analytically. For a sum over polarization the approach is still advantageous, but with an integration over an unobserved momentum, as in $d^2\sigma$, it is not.

Here we chose the photon momentum $\vec{k}$ (energy $k=|\vec{k}|$) along the $z$ axis, and the incident electron momentum in the $x$-$z$ plane. In this coordinate system, we choose $a^{\uparrow},a^{\downarrow}$ as the complex coefficients of the decomposition of the electron spinors into spin up and down eigenvectors along the $z$ axis in the rest system of each electron. We choose $\epsilon_+,\epsilon_-$ as the complex polarization coefficients of the decomposition of the photon polarization into left and right circular polarization with respect to the $z$ axis. The matrix element can be written as

$$M_{f,i}=M_{\uparrow\uparrow+}a_1^{\uparrow}a_2^{\uparrow*}\epsilon_+^*+M_{\uparrow\uparrow-}a_1^{\uparrow}a_2^{\uparrow*}\epsilon_-^*+M_{\uparrow\downarrow+}a_1^{\uparrow}a_2^{\downarrow*}\epsilon_+^* + \cdots=\sum_{n=1}^{8}M_n v_n=\sum_{\mathscr{L}}\mathscr{M}_{\mathscr{L}}, \tag{1}$$

where for convenience in later discussion we label the matrix elements in Eq. (1) as $M_1=M_{\uparrow\uparrow+}$, $M_2=M_{\uparrow\uparrow-}$, . . . ,$M_8=M_{\downarrow\downarrow-}$ and the spin polarization coefficients as $v_1=a_1^{\uparrow}a_2^{\uparrow*}\epsilon_+^*$, $v_2=a_1^{\uparrow}a_2^{\uparrow*}\epsilon_-^*$, . . . , $v_8=a_1^{\downarrow}a_2^{\downarrow*}\epsilon_-^*$. We obtain the $M_n$ by summing the numerical results calculated for each $\mathscr{L}$ using Tseng's original code. The triply differential cross section can be written as

$$d^3\sigma\equiv\frac{d^3\sigma}{dk\,d\Omega_k d\Omega_e}=C_0\sum_{m,n=1}^{8}v_m^*M_m^*M_n v_n =C_0\sum_{m,n=1}^{8}v_m^*D_{m,n}v_n, \tag{2}$$

with $D_{m,n}=M_m^*M_n$. Here the constant $C_0$ is a function of electron and photon energies determined by the choice of normalization of the electron spinors and photon wave function in the matrix element (1). Note that both the $v_n$ and the $M_n$ are complex numbers. All the information on the polarization correlations is included in the matrix $D$. Given $D$, if we specify the state vectors $v_n$, we can easily calculate the cross section for the corresponding process. If we do not observe any polarization information, we can obtain the unpolarized triply differential cross section by averaging over the polarization of the initial electron and summing over the polarization of the final electron and radiated photon, obtaining

$$\frac{d^3\sigma_{\mathrm{unpol}}}{dk d\Omega_k d\Omega_e} = \frac{1}{2} C_0 \sum_{i=1}^{8} D_{ii} = \frac{1}{2} C_0 \sum_{i=1}^{8} |M_i|^2. \tag{3}$$

To facilitate comparison with other existing experimental data, we introduce quantities $C_{200}$ and $P$, corresponding to two types of experimental measurements which involve use of a polarized electron beam or observation of photon polarization. The first of these experiments is the so-called ''photon emission asymmetry'' measurement ($C_{200}$ in the language of Pratt and Feng [7]), where coincidence events are counted for fixed outgoing photon and electron angle (without determining the polarization of the final state electron or photon), with the incident electron beam polarization (as measured in the rest frame of the electron) normal to the scattering plane, either ''up'' (in the $\vec{k}\times\vec{p}_i$ direction), denoted $\uparrow$, or ''down'' ($\downarrow \equiv -\uparrow$). Assuming a perfectly polarized beam,

$$C_{200} = \frac{n^{\uparrow} - n^{\downarrow}}{n^{\uparrow} + n^{\downarrow}}, \tag{4}$$

where $n^{\uparrow}$ and $n^{\downarrow}$ represent the number of coincidence events with the incident beam polarized ''up'' and ''down,'' respectively. In our notation

$$C_{200} = \frac{d^3\sigma^{\uparrow} - d^3\sigma^{\downarrow}}{d^3\sigma^{\uparrow} + d^3\sigma^{\downarrow}}, \tag{5}$$

where

$$d^3\sigma^{\pm\uparrow} = \frac{C_0}{2} \sum_{n=1}^{4} |M_n \pm i M_{n+4}|^2. \tag{6}$$

We note that $C_{200}$ vanishes in the lowest order Born approximation. The second ''polarization observable'' for which experiments exist is photon linear polarization where, using an unpolarized incident electron beam and not determining the polarization of the outgoing electrons, the intensity of emission of photons with polarization perpendicular or parallel to the scattering plane is measured. The polarization

$$P = \frac{I_{\perp} - I_{\parallel}}{I_{\perp} + I_{\parallel}}. \tag{7}$$

In our notation

$$P = \frac{d^3\sigma_+ - d^3\sigma_-}{d^3\sigma_+ + d^3\sigma_-}, \tag{8}$$

where

$$d^3\sigma_{\pm} = \frac{C_0}{2} \sum_{n=1}^{4} |M_{2n-1} \pm M_{2n}|^2. \tag{9}$$

Testing of our code has included comparing predictions for low $Z$ and high energy with predictions of the Bethe-Heitler theory, checking for partial-wave and multipole convergence and comparison of numerical integration of $d^3\sigma$ with $d^2\sigma$ calculated using analytic integration. The cases selected for comparison with simpler theories were those with parameters similar to existing experiments as well as some additional tests where ''gaps'' appeared. The tests include $Z=1,3,6,13,29$ with energies in the range of hundreds of keV. In all these cases the Bethe-Heitler results have been reproduced within their expected accuracy. For higher $Z$ (29, 33, 47), limited additional verification has been achieved by comparison with Elwert-Haug results, again reproducing the results of this theory within acceptable tolerances. Numerical convergence of the partial-wave and multipole series has been tested by monitoring the size and rate of decrease of the contribution of the higher partial waves. In cases where convergence is slow, particularly for small values of $k/E_1$, our data are not presented. The results presented here should be accurate to better than 1%. Finally, for a sample $Z=6$ case, $d^3\sigma$ was calculated for a ''grid'' of outgoing electron angles and integrated numerically. This result was then compared to Tseng's result for $d^2\sigma$ which was obtained by integrating analytically over outgoing angles [6]. The numerical and analytic results agreed within 5%, which is acceptable for the selected grid spacing.

## III. RESULTS AND DISCUSSION

### A. Results

It is convenient, for comparison with experimental data, to define the angles $\theta_e$ and $\theta_\gamma$, which are the outgoing electron and photon polar angles measured relative to the incident electron momentum vector. In these calculations we focus on comparisons with simpler theories, but in anticipation of new data we have selected parameters corresponding to experiments that have already been performed [10–12]. For reference we present in Table I the relevant parameters for all high-$Z$ experiments of which we are aware. Table I also contains a qualitative description of how our results compare with Elwert-Haug predictions and with experiment. In the comparison with Elwert and Haug, ''fair'' and ''poor'' indicate agreement better and worse, respectively, than 20% for most values of the relevant parameters. In the comparisons with experiment, ''good,'' ''fair,'' and ''poor'' indicate agreement within three standard deviations for all, most, and few values, respectively, of the relevant parameters. While we have performed calculations for all of the cases in Table I, in some instances slow convergence in the partial-wave series led us to forgo making assessments of the agreement among theory and experiments at this time. An example of our cross section results, together with predictions from the theory of Elwert and Haug and experimental data, are displayed in Fig. 1 (corresponding to Fig. 3 of [10]). Here the cross section for $E_1=300$ keV, $Z=79$, $\theta_e=0°$, and $\theta_\gamma=20°$ was calculated as a function of outgoing photon energy. As with all currently existing experiments, coplanar geometry is used. The Elwert-Haug predictions are given in the experimental papers; we have verified the values by making a direct numerical calculation. Figure 2 displays a further example of our cross section calculations, Elwert-Haug re-

TABLE I. Available experimental data and qualitative assessment of the comparison of Elwert-Haug (EH) predictions and experiment with our results. This table does not give a complete description of the listed experiments but identifies all experiments which involved targets with $Z \geqslant 47$. In the comparison with Elwert-Haug results, ''fair'' and ''poor'' indicate agreement better and worse, respectively, than 20% for most values of the relevant parameters. In the comparisons with experiment, ''good,'' ''fair,'' and ''poor'' indicate agreement within three standard deviations for all, most, and few values, respectively, of the relevant parameters. ''NA'' indicates cases for which our results are not yet available. The types of experiments are described in the text.

| Ref. | $Z$ | Type | $E_1$ (keV) | $E_2$ (keV) | $\theta_e$ | $\theta_\gamma$ | EH | Experiment |
|---|---|---|---|---|---|---|---|---|
| [13] | 47 | $d^3\sigma$ | 180 | 100 | 30° | $-80° \rightarrow 60°$ | fair | fair |
| [11] | 47 | $d^3\sigma$ | 300 | 50–200[a] | −20° | 35° | fair | good |
| [16] | 79 | $d^3\sigma$ | 140 | 20–70 | 15°,30° | 30°,270° | poor | fair |
| [11] | 79 | $d^3\sigma$ | 300 | 50–200 | −20° | 35° | fair | fair |
| [10] | 79 | $d^3\sigma$[b] | 300 | 69–249 | 0°,20° | 10°,20° | fair | fair |
| [17] | 79 | $d^3\sigma$ | 300 | 170 | 0°,5° | $-40° \rightarrow 40°$ | NA | NA |
| [12] | 79 | $C_{200}$ | 300 | 160, 200 | 0°,20°,45°[c] | $-60° \rightarrow 0°$ | fair | good |
| [18] | 79 | $P$ | 300 | 140 | 20° | $-40° \rightarrow 20°$[d] | NA | NA |

[a]A total of eight experimental data points were collected over this range of energies.
[b]Only relative cross sections were obtained in this experiment.
[c]Five or fewer experimental data points (photon emission angles) available for each value of $\theta_e$.
[d]Five experimental data points.

sults and experimental data from Fig. 3 of [13]. In this case the data are displayed for $E_1=180$ keV, $E_2=100$ keV, $Z=47$, and $\theta_e=30°$ as a function of $\theta_\gamma$. Finally, in Fig. 3 we present data for the photon emission asymmetry compared with experimental results from Fig. 2 of [12]. These data correspond to $E_1=300$ keV, $Z=79$, $k=100$ keV, and $\theta_e=20°$, as a function of $\theta_\gamma$.

### B. Comparison with other theories

While systematic comparisons of the various theories for $d^3\sigma$ are yet to be undertaken, we can make some comments based on the calculations performed thus far. Since it is expected that Elwert-Haug and Bethe-Heitler [14] predictions should be adequate to describe the intermediate- and low-$Z$ regime we have selected high-$Z$ cases for our initial studies. Aside from the tests described in Sec. II, all of our initial calculations have concentrated on these high-$Z$ cases (see Table I). For the high atomic numbers considered here we find that the Bethe-Heitler results, while giving the correct qualitative features of the angular distribution and spectrum, predict cross sections differing quantitatively from ours by more than 100% in many cases. This is not surprising, since the $Z\alpha/\beta \ll 1$ criteria for the validity of the Bethe-Heitler result are not satisfied here. There is also very little reason to expect the Elwert-Haug results to be correct for these cases.

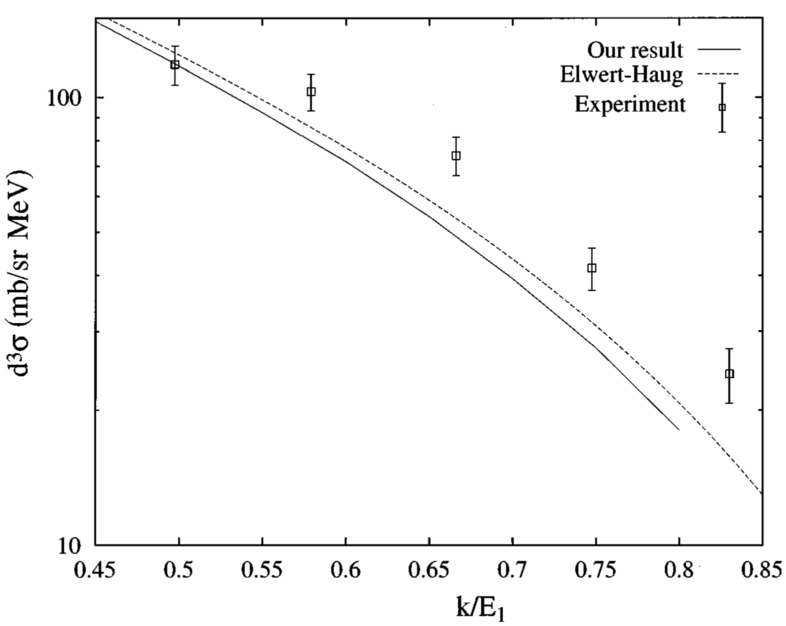


FIG. 1. Triply differential cross section for $E_1=300$ keV, $Z=79$, $\theta_e=0°$, and $\theta_\gamma=20°$, as a function of the fraction $k/E_1$ of incident electron energy radiated by the photon. We show our predictions, Elwert-Haug predictions including form factors, and experimental data. The experimental data are from Fig. 4 of [10].

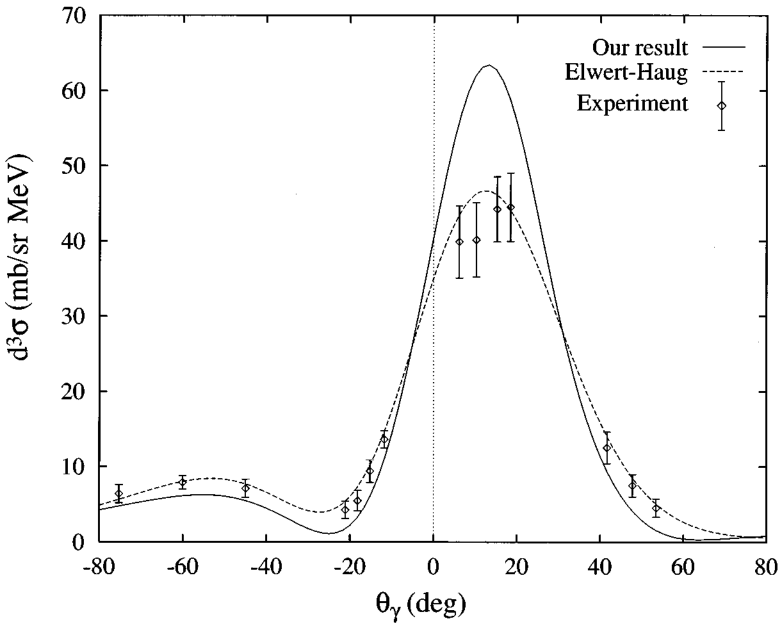


FIG. 2. Triply differential cross section for $E_1 = 180$ keV, $E_2 = 100$ keV, $Z = 47$, and $\theta_e = 30°$, as a function of photon angle. We compare our predictions, Elwert-Haug results including form factors, and experiment. The experimental data are from Fig. 3 of [13].

(Note that in Born approximation $C_{200}$ vanishes, so the entire polarization effect reflects the deviation from Born approximation.)

Figure 1 is a typical example of a spectrum for fixed detector geometry. (While in this particular geometry Elwert-Haug results are larger than ours, Fink and Pratt [15] have reported that for $d^2\sigma$ Elwert-Haug results are systematically smaller than the exact partial-wave results of Tseng. We can conclude that the outgoing electron angles chosen for Fig. 1 are not the dominant ones in the integrated cross sections.) In some cases, particularly for the $Z = 47$ and the $C_{200}$ cases, as displayed in Figs. 2 and 3, the agreement between these two theories could be described as "fair." While the Elwert-Haug results approach the correct high-$Z$, high energy limit (in the then dominant small angle regions) [3], until more systematic studies are completed it is unclear at what energies or angles these results begin to be correct. From our existing data it appears that the Elwert-Haug theory is still performing reasonably well for $Z = 47$ at relatively low energies (much lower than those required for high energy limit behavior to prevail). Additionally, we find that even for $Z = 79$ the Elwert-Haug predictions for the polarization observable $C_{200}$ appear to be close to ours in the cases we have studied.

### C. Comparison with experiments

Qualitative descriptions of the agreement of our theory with all published high-$Z$ experimental data are given in Table I. It should be noted that our calculations do not directly account for experimental corrections such as finite detector size and resolution. The significance of these corrections was estimated by comparing our Elwert-Haug results with Elwert-Haug results which include such corrections,

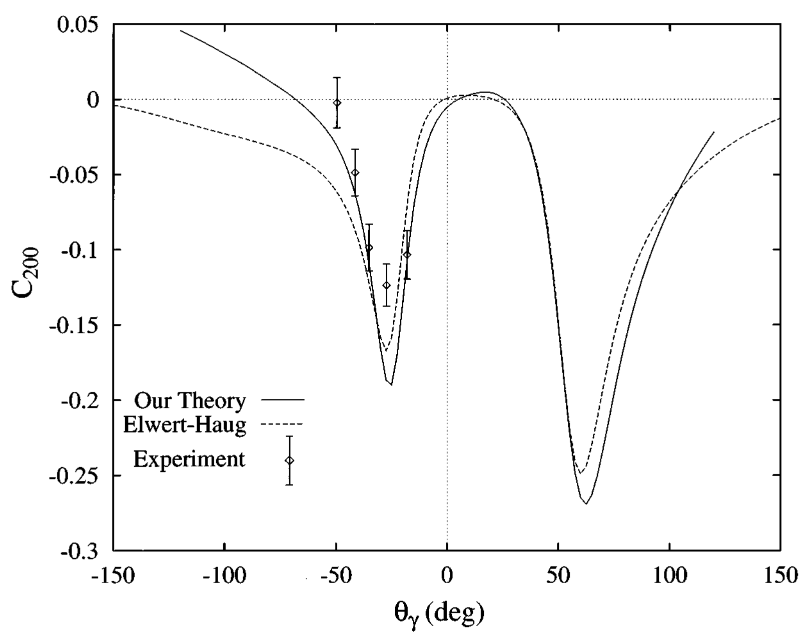


FIG. 3. Photon emission asymmetry, $C_{200}$, for $E_1 = 300$ keV, $E_2 = 200$ keV, and $\theta_e = 20°$, as a function of photon angle. We compare our predictions, Elwert-Haug results, and experiment. The experimental data are from Fig. 2 of [12].

whenever they are presented in the experimental papers. In all such cases the effect of these corrections was small. Figure 1 is representative of the lack of agreement found in many of the $Z=79$ cases. Figure 2 provides an example for $Z=47$ where some agreement between our theory and experiment is achieved. In this case, some significant discrepancies are seen near the largest peak of the angular distribution (where a large number of partial waves were required to obtain convergence in our result), while away from this peak fairly good agreement is found. As a final example, we find relatively good agreement (see Fig. 3) with the $C_{200}$ experiment of Mergl *et al.* [12].

## IV. SUMMARY

Calculations for the triply differential cross section $d^3\sigma$ in bremsstrahlung, using our code, have been performed over ranges of parameters corresponding to previously existing experiments. In particular, we have concentrated on those experiments with $Z\geqslant 47$ and electron energies in the 100 keV region where none of the previously existing theories was expected to perform well. For these cases we find no systematic agreement yet with the simpler Elwert-Haug theory. The cases where marginal agreement can been seen in the cross section are predominantly those with $Z=47$. Some agreement at $Z=79$ was found in the predictions of the photon emission asymmetry ($C_{200}$) calculated under the conditions listed in Table I. Comparison of our predictions with the experimental data yields similar results. For cross sections we find some agreement with experiment for the $Z=47$ cases, while we find fairly poor agreement for higher $Z$. Also we see some agreement between our results for the photon emission asymmetry ($C_{200}$) at $Z=79$ and those of experiment. We tend to agree with the presently available experimental data whenever we also agree well with the previously available Elwert-Haug predictions. In cases where large discrepancies are seen between our results and those of Elwert and Haug, the experimental data do not systematically support either theory. It is hoped that future, more accurate, experiments will help to clarify discrepancies between theory and experiment.

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